A consensus yeast metabolic network reconstruction obtained from a community approach to systems biology

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Published in:
Nature Biotechnology

DOI:
10.1038/nbt1492

Supplementary Figure 1. An example of some of the SBML annotations of compartments, species and reactions, using the example of the reaction catalyzed by the gene product hexokinase 2 of the *HXK2* gene, as used in the reconstruction of the consensus network, illustrating its use of the Systems Biology Ontology (http://www.ebi.ac.uk/sbo/) and its MIRIAM-compliance.

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http://www.sbml.org/sbml/level2/version3" level="2"
version="3">
  <model metaid="metaid_ymn1_0" id="ymn1_0" name="Yeast metabolic network">
    <notes>
      <body xmlns="http://www.w3.org/1999/xhtml">
        <p>This is a reconstruction of the biochemical network of the yeast
        <i>Saccharomyces cerevisiae</i> carried out at a jamboree organized
in April 2007 in the Manchester Centre for Integrative Systems Biology. It
is the result of a consensus merger of two previous reconstructions.</p>
        <p>Technical notes:

        <ul>
          <li>The compartments included here have no volume defined; there
are no reliable estimates available for those volumes yet.</li>
          <li>There are no kinetic functions defined for the reactions
because this model only represents the chemical structure of the network
(stoichiometry).</li>
          <li>All reactions are marked reversible because all chemical
reactions are reversible.</li>
        </ul>
      </p>
      <p>This SBML representation of the yeast metabolic network is made
available under the Creative Commons Attribution-Share Alike 3.0 Unported
Licence (see
      <a
href="http://www.creativecommons.org">www.creativecommons.org</a>).</p>
    </body>
  </notes>
  <annotation>
    <rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
xmlns:dc="http://purl.org/dc/elements/1.1/"
xmlns:dcterms="http://purl.org/dc/terms/"
xmlns:vCard="http://www.w3.org/2001/vcard-rdf/3.0#"
xmlns:bqbiol="http://biomodels.net/biology-qualifiers/"
xmlns:bqmodel="http://biomodels.net/model-qualifiers/">
      <rdf:Description rdf:about="#metaid_ymn1_0">
        <dc:creator rdf:parseType="Resource">
          <rdf:Bag>
            <rdf:li rdf:parseType="Resource">
              <vCard:N rdf:parseType="Resource">
                <vCard:Family>Herrgard</vCard:Family>
                <vCard:Given>Markus</vCard:Given>
              </vCard:N>
              <vCard:EMAIL>mherrgar@ucsd.edu</vCard:EMAIL>
              <vCard:ORG>
                <vCard:Orgname>University of California, San
Diego</vCard:Orgname>
              </vCard:ORG>
            </rdf:li>
            <rdf:li rdf:parseType="Resource">
              <vCard:N rdf:parseType="Resource">
                <vCard:Family>Swainston</vCard:Family>
```

```
              <vCard:Given>Neil</vCard:Given>
            </vCard:N>
            <vCard:EMAIL>neil.swainston@manchester.ac.uk</vCard:EMAIL>
            <vCard:ORG>
              <vCard:Orgname>University of Manchester</vCard:Orgname>
            </vCard:ORG>
          </rdf:li>
        </rdf:Bag>
      </dc:creator>
      <dcterms:created rdf:parseType="Resource">
        <dcterms:W3CDTF>2008-02-20T10:05:10Z</dcterms:W3CDTF>
      </dcterms:created>
      <dcterms:modified rdf:parseType="Resource">
        <dcterms:W3CDTF>2008-05-15T17:52:27Z</dcterms:W3CDTF>
      </dcterms:modified>
      <bqbiol:is>
        <rdf:Bag>
          <rdf:li rdf:resource="urn:miriam:taxonomy:4932"/>
        </rdf:Bag>
      </bqbiol:is>
    </rdf:Description>
  </rdf:RDF>
 </annotation>
⋮
 <listOfCompartments>
  <compartment metaid="metaid_C_1" id="C_1" name="Cytoplasm" outside="C_10"
sboTerm="SBO:0000290">
    <annotation>
      <rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
xmlns:dc="http://purl.org/dc/elements/1.1/"
xmlns:dcterms="http://purl.org/dc/terms/"
xmlns:vCard="http://www.w3.org/2001/vcard-rdf/3.0#"
xmlns:bqbiol="http://biomodels.net/biology-qualifiers/"
xmlns:bqmodel="http://biomodels.net/model-qualifiers/">
        <rdf:Description rdf:about="#metaid_C_4">
          <bqbiol:is>
            <rdf:Bag>
              <rdf:li rdf:resource="urn:miriam:obo.go:GO:0005737"/>
            </rdf:Bag>
          </bqbiol:is>
        </rdf:Description>
      </rdf:RDF>
    </annotation>
  </compartment>
⋮
 </listOfCompartments>
 </listOfSpecies>
⋮
  <species metaid="metaid_M_172" id="M_172" name="ATP" compartment="C_1"
sboTerm="SBO:0000299">
    <annotation>
      <in:inchi xmlns:in="http://biomodels.net/inchi" metaid="M_172_inchi">
InChI=1/C10H16N5O13P3/c11-8-5-9(13-2-12-8)15(3-14-5)10-7(17)6
(16)4(26-10)1-25-30(21,22)28-31(23,24)27-29(18,19)20/h2-4,6-7,10,16-17H,1H2,
(H,21,22)(H,23,24)(H2,11,12,13)(H2,18,19,20)/t4-,6-,7-,10-/m1/s1/f/h18-19,21
,23H,11H2
      </in:inchi>
      <rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
```

```
xmlns:dc="http://purl.org/dc/elements/1.1/"
xmlns:dcterms="http://purl.org/dc/terms/"
xmlns:vCard="http://www.w3.org/2001/vcard-rdf/3.0#"
xmlns:bqbiol="http://biomodels.net/biology-qualifiers/"
xmlns:bqmodel="http://biomodels.net/model-qualifiers/">
          <rdf:Description rdf:about="#metaid_M_172">
            <bqbiol:is>
              <rdf:Bag>
                <rdf:li rdf:resource="urn:miriam:obo.chebi:CHEBI:15422"/>
                <rdf:li rdf:resource="#M_172_inchi"/>
              </rdf:Bag>
            </bqbiol:is>
          </rdf:Description>
        </rdf:RDF>
      </annotation>
    </species>
⋮
    <species metaid="metaid_E_450" id="E_450" name="YCL040W"
compartment="C_1" sboTerm="SBO:0000014">
      <annotation>
        <rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
xmlns:dc="http://purl.org/dc/elements/1.1/"
xmlns:dcterms="http://purl.org/dc/terms/"
xmlns:vCard="http://www.w3.org/2001/vcard-rdf/3.0#"
xmlns:bqbiol="http://biomodels.net/biology-qualifiers/"
xmlns:bqmodel="http://biomodels.net/model-qualifiers/">
          <rdf:Description rdf:about="#metaid_E_450">
            <bqbiol:is>
              <rdf:Bag>
                <rdf:li rdf:resource="urn:miriam:sgd:S000000545"/>
                <rdf:li rdf:resource="urn:miriam:uniprot:P17709"/>
              </rdf:Bag>
            </bqbiol:is>
          </rdf:Description>
        </rdf:RDF>
      </annotation>
    </species>
⋮
  </listOfSpecies>
  </listOfReactions>
⋮
    <reaction metaid="metaid_R_1550" id="R_1550" name="hexokinase
(D-glucose:ATP)" sboTerm="SBO:0000176">
      <notes>
        <html xmlns="http://www.w3.org/1999/xhtml">
          <p>SUBSYSTEM: Glycolysis/Gluconeogenesis</p>
        </html>
      </notes>
      <annotation>
        <rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
xmlns:dc="http://purl.org/dc/elements/1.1/"
xmlns:dcterms="http://purl.org/dc/terms/"
xmlns:vCard="http://www.w3.org/2001/vcard-rdf/3.0#"
xmlns:bqbiol="http://biomodels.net/biology-qualifiers/"
xmlns:bqmodel="http://biomodels.net/model-qualifiers/">
          <rdf:Description rdf:about="#metaid_R_1550">
            <bqbiol:is>
              <rdf:Bag>
```

```
              <rdf:li rdf:resource="urn:miriam:ec-code:2.7.1.2"/>
            </rdf:Bag>
          </bqbiol:is>
          <bqmodel:isDescribedBy>
            <rdf:Bag>
              <rdf:li rdf:resource="urn:miriam:pubmed:6394965"/>
            </rdf:Bag>
          </bqmodel:isDescribedBy>
        </rdf:Description>
      </rdf:RDF>
    </annotation>
    <listOfReactants>
      <speciesReference species="M_172"/>
      <speciesReference species="M_304"/>
    </listOfReactants>
    <listOfProducts>
      <speciesReference species="M_135"/>
      <speciesReference species="M_292"/>
      <speciesReference species="M_329"/>
    </listOfProducts>
    <listOfModifiers>
      <modifierSpeciesReference species="E_450"/>
    </listOfModifiers>
  </reaction>
⋮
 </listOfReactions>
</model>
</sbml>
```